EP 2 472 270 A1 20120704

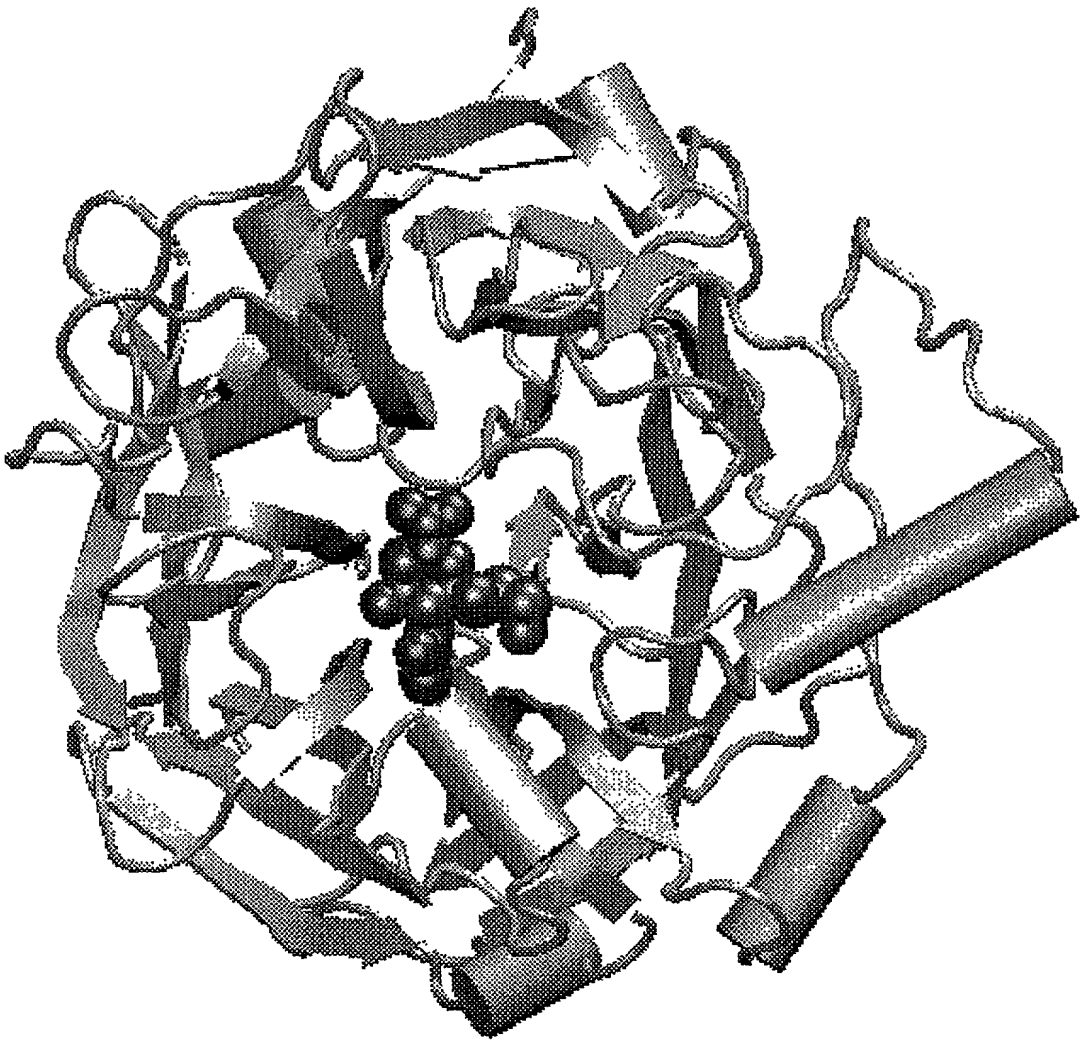
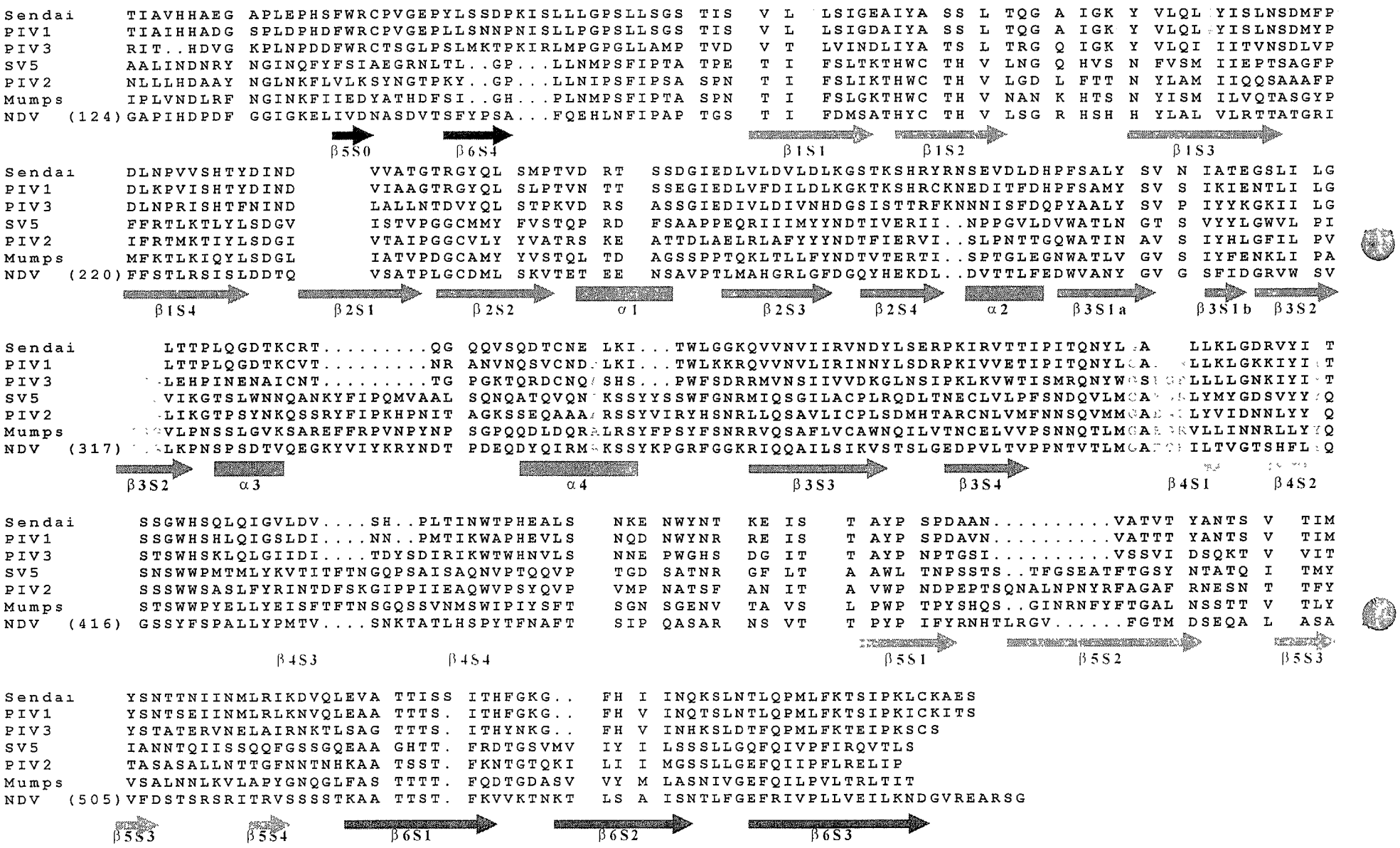


Fig. 1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PIV1 TIAIHHADG SPLDPHDFWRCPVGEPLLSNNPNISLLPGPSLLSGS TIS V L LSIGDAIYA SS L TQG A IGK Y VLQL YISLNSDMYP
PIV3 RIT..HDVG KPLNPDDFWRCTSGLPSLMKTPKIRLMPGPGLLAMP TVD V T LVINDLIYA TS L TRG Q IGK Y VLQI IITVNSDLVP
SV5 AALINDNRY NGINQFYFSIAEGRNLTL..GP...LLNMPSFIPTA TPE T I FSLTKTHWC TH V LNG Q HVS N FVSM IIEPTSAGFP
PIV2 NLLLHDAAY NGLNKFLVLKSYNGTPKY..GP...LLNIPSFIPSA SPN T I FSLIKTHWC TH V LGD L FTT N YLAM IIQQSAAAFP
Mumps IPLVNDLRF NGINKFIIEDYATHDFSI..GH...PLNMPSFIPTA SPN T I FSLGKTHWC TH V NAN K HTS N YISM ILVQTASGYP
NDV (124) GAPIHDPDF GGIGKELIVDNASDVTSFYPSA...FQEHLNFIPAP TGS T I FDMSATHYC TH V LSG R HSH H YLAL VLRTTATGRI
β5S0
β6S4
β1S1
β1S2
β1S3
Sendai DLNPVVSHTYDIND VVATGTRGYQL SMPTVD RT SSDGIEDLVLDVLDLKGSTKSHRYRNSEVDLDHPFSALY SV N IATEGSLI LG
PIV1 DLKPVISHTYDIND VIAAGTRGYQL SLPTVN TT SSEGIEDLVFDILDLKGKTKSHRCKNEDITFDHPFSAMY SV S IKIENTLI LG
PIV3 DLNPRISHTFNIND LALLNTDVYQL STPKVD RS ASSGIEDIVLDIVNHDGSISTTRFKNNNISFDQPYAALY SV P IYYKGKII LG
SV5 FFRTLKTLYLSDGV ISTVPGGCMMY FVSTQP RD FSAAPPEQRIIIMYYNDTIVERII..NPPGVLDVWATLN GT S VYYLGWVL PI
PIV2 IFRTMKTIYLSDGI VTAIPGGCVLY YVATRS KE ATTDLAELRLAFYYYNDTFIERVI..SLPNTTGQWATIN AV S IYHLGFIL PV
Mumps MFKTLKIQYLSDGL IATVPDGCAMY YVSTQL TD AGSSPPTQKLTLLFYNDTVTERTI..SPTGLEGNWATLV GV S IYFENKLI PA
NDV (220) FFSTLRSISLDDTQ VSATPLGCDML SKVTET EE NSAVPTLMAHGRLGFDGQYHEKDL..DVTTLFEDWVANY GV G SFIDGRVW SV
β1S4
β2S1
β2S2
α1
β2S3
β2S4
α2
β3S1a
β3S1b
β3S2
Sendai LTTPLQGDTKCRT.....QG QQVSQDTCNE LKI...TWLGGKQVVNVIIRVNDYLSERPKIRVTTIPITQNYL A LLKLGDRVYI T
PIV1 LTTPLQGDTKCVT.....NR ANVNQSVCND LKI...TWLKKRQVVNVLIRINNYLSDRPKIVVETIPITQNYL A LLKLGKKIYI T
PIV3 LEHPINENAICNT.....TG PGKTQRDCNQ SHS...PWFSDRRMVNSIIVVDKGLNSIPKLKVWTISMRQNYW S LLLLGNKIYI T
SV5 VIKGTSLWNNQANKYFIPQMVAAL SQNQATQVQN KSSYYSSWFGNRMIQSGILACPLRQDLTNECLVLPFSNDQVLMC A LYMYGDSVYY Q
PIV2 LIKGTPSYNKQSSRYFIPKHPNIT AGKSSEQAAA RSSYVIRYHSNRLLQSAVLICPLSDMHTARCNLVMFNNSQVMM A LYVIDNNLYY Q
Mumps VLPNSSLGVKSAREFFRPVNPYNP SGPQQDLDQR LRSYFPSYFSNRRVQSAFLVCAWNQILVTNCELVVPSNNQTLM A RVLLINNRLLY Q
NDV (317) LKPNSPSDTVQEGKYVIYKRYNDT PDEQDYQIRM KSSYKPGRFGGKRIQQAILSIKVSTSLGEDPVLTVPPNTVTLM A ILTVGTSHFL Q
β3S2
α3
α4
β3S3
β3S4
β4S1
β4S2
Sendai SSGWHSQLQIGVLDV....SH..PLTINWTPHEALS NKE NWYNT KE IS T AYP SPDAAN.....VATVT YANTS V TIM
PIV1 SSGWHSHLQIGSLDI....NN..PMTIKWAPHEVLS NQD NWYNR RE IS T AYP SPDAVN.....VATTT YANTS V TIM
PIV3 STSWHSKLQLGIIDI....TDYSDIRIKWTWHNVLS NNE PWGHS DG IT T AYP NPTGSI.....VSSVI DSQKT V VIT
SV5 SNSWWPMTMLYKVTITFTNGQPSAISAQNVPTQQVP TGD SATNR GF LT A AWL TNPSSTS..TFGSEATFTGSY NTATQ I TMY
PIV2 SSSWWSASLFYRINTDFSKGIPPIIEAQWVPSYQVP VMP NATSF AN IT A VWP NDPEPTSQNALNPNYRFAGAF RNESN T TFY
Mumps STSWWPYELLYEISFTFTNSGQSSVNMSWIPIYSFT SGN SGENV TA VS L PWP TPYSHQS..GINRNFYFTGAL NSSTT V TLY
NDV (416) GSSYFSPALLYPMTV....SNKTATLHSPYTFNAFT SIP QASAR NS VT T PYP IFYRNHTLRGV.....FGTM DSEQA L ASA
β4S3
β4S4
β5S1
β5S2
β5S3
Sendai YSNTTNIINMLRIKDVQLEVA TTISS ITHFGKG.. FH I INQKSLNTLQPMLFKTSIPKLCKAES
PIV1 YSNTSEIINMLRLKNVQLEAA TTTS. ITHFGKG.. FH V INQTSLNTLQPMLFKTSIPKICKITS
PIV3 YSTATERVNELAIRNKTLSAG TTTS. ITHYNKG.. FH V INHKSLDTFQPMLFKTEIPKSCS
SV5 IANNTQIISSQQFGSSGQEAA GHTT. FRDTGSVMV IY I LSSSLLGQFQIVPFIRQVTLS
PIV2 TASASALLNTTGFNNTNHKAA TSST. FKNTGTQKI LI I MGSSLLGEFQIIPFLRELIP
Mumps VSALNNLKVLAPYGNQGLFAS TTTT. FQDTGDASV VY M LASNIVGEFQILPVLTRLTIT
NDV (505) VFDSTSRSRITRVSSSSTKAA TTST. FKVVKTNKT LS A ISNTLFGEFRIVPLLVEILKNDGVREARSG
β5S3
β5S4
β6S1
β6S2
β6S3

Figure 2

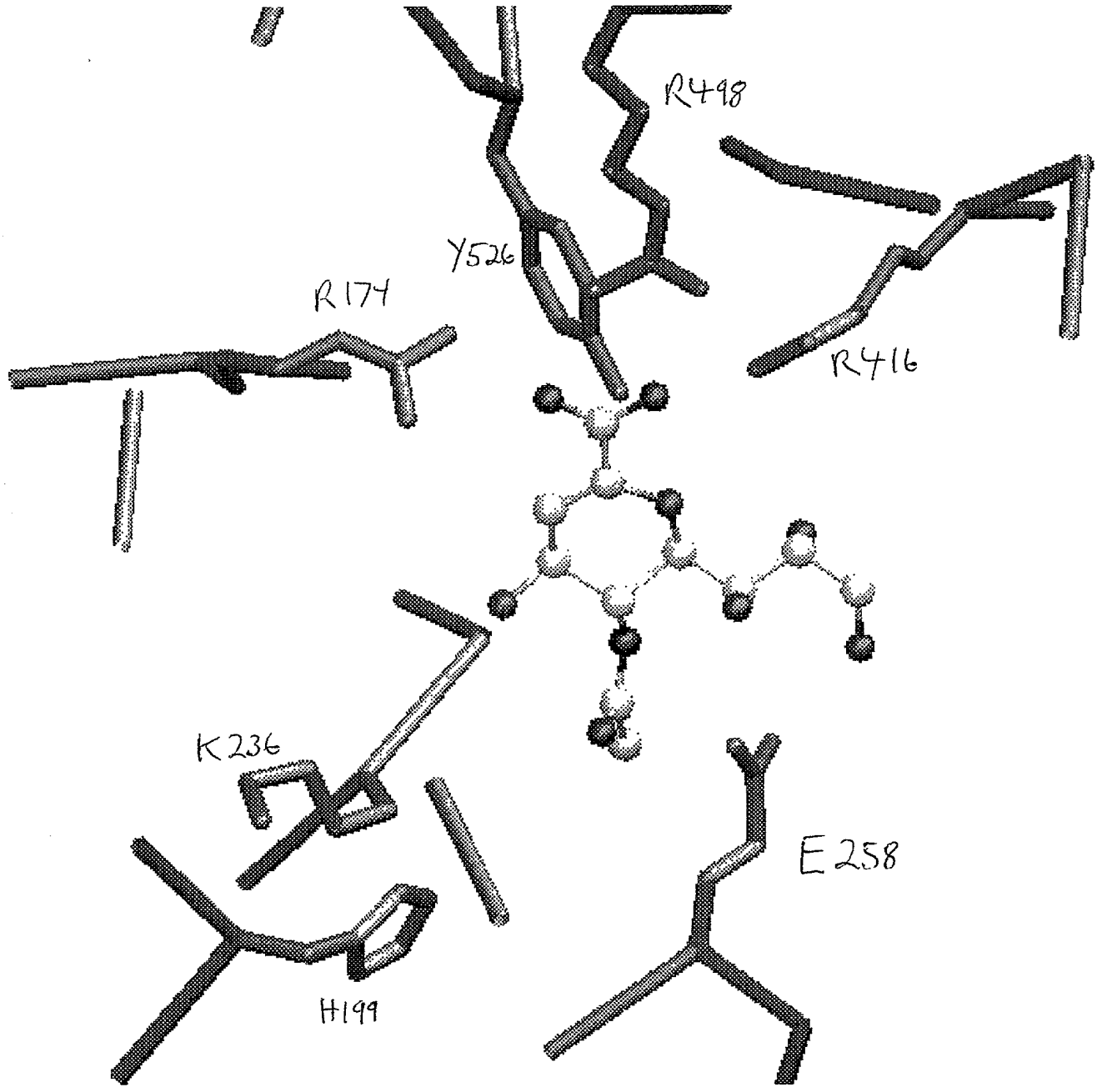

Fig. 3

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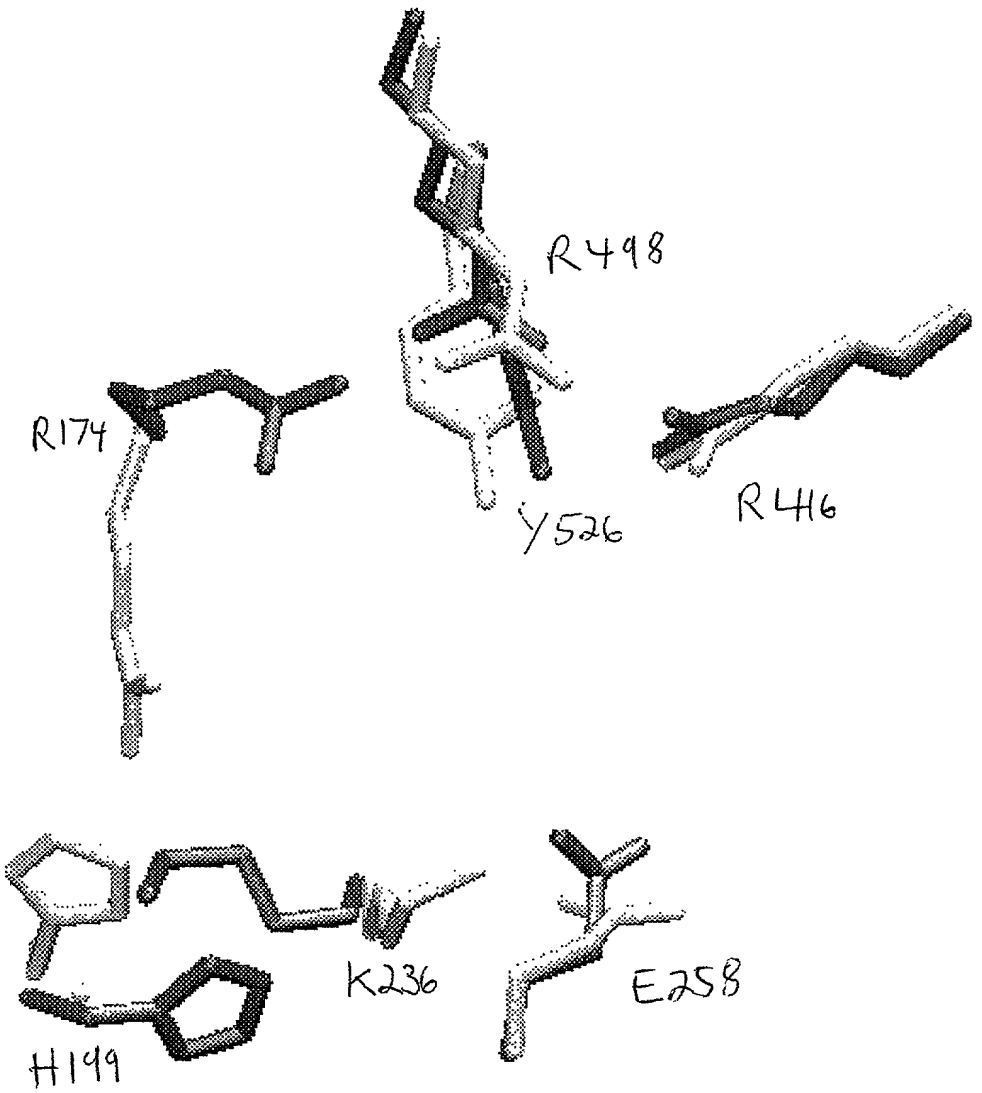

Fig. 4

	Native 1	Native 2	Native 3	Native 4	NANA	DANA
Cell (Å)	73.3	72.3	71.7	72.0	71.6	137.5
	78.0	77.9	77.9	83.8	77.6	137.5
	202.6	199.2	198.2	201.5	197.2	116.6
Temp(K), pH	293, 7	100, 4.6	100, 4.6	293, 6	100K, 4.6	100K,6.5
Resolution (Å)	3.0	2.0	2.5	3.0	2.5	2.8
# obs	172104	623166	420703	277932	210555	498619
# unique	20022	68217	38168	22207	29671	38673
Completeness(%)	83	86	97	88	76	94
R_{merg} (%)	9.3	4.9	3.1	9.3	4.2	5.2
R-factor			0.222		.223	0.209
R_{free}			0.277		.291	0.235
# protein atoms			6914		6914	6896
# CHO, Ca,			89		116	111

Fig. 5

09/15/15 - 09/25/04

ligands			
# waters	211	207	239
<B> A, B Å^2	25,36	32,44	44,44
<B> ligand Å^2		38,57	48,41

Table 1 Crystallographic data and refinement statistics.

Datasets Native2, Native3, NANA and DANA from frozen crystals were collected on beamlines X11 and BW7A at DESY, Hamburg. All other datasets were collected on in-house rotating anode and image plate or multiwire detector systems.

$R_{merge} = \Sigma_{hkl} \Sigma_i |\Sigma I^i_{hkl} - \langle I_{hkl} \rangle| / \Sigma_{hkl} \Sigma_i \langle I^i_{hkl} \rangle$ where the sum *i* is over all separate measurements of the unique reflections hkl.

$R\text{-factor} = \Sigma_{hkl} ||F_{obs}| - |F_{calc}|| / \Sigma_{hkl} |F_{obs}|$

R_{free}, as R-factor but summed over a 10% test set of reflections.

Fig. 5 (continued)